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Molecular Shape and VSEPR Theory

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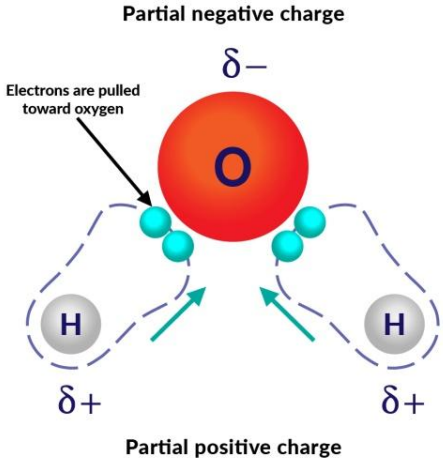
Polarity of Molecules

Molecules are groups of atoms held together by _____ bonds. These bonds may be polar or non-polar. (See lesson 2-2 on covalent bonding for more details on polar and non-polar bonding)

Polar Molecules

Recall that polar bonds result in one side of the molecule having a slightly positive electrical charge (_____), while the other has a slightly negative charge (_____). These molecules are called polar molecules.



The polarity of a molecule depends on:

- The molecule containing _____ bonds
- The polar bonds in the molecule being arranged _____ around the central atom e.g. water _____ or ammonia _____. In molecules such as water, the most electronegative atom (in the case of water, oxygen) pulls the electrons towards itself and away from the other atoms. This makes the oxygen partially negative due to the presence of the electrons from the hydrogen.
- More than one type of atom bonded to a central atom (e.g. trichloromethane $CHCl_3$)
- The centers of positive and negative charge not coinciding.

Non-polar Molecules

A non-polar molecule has no overall electrical _____. There are two types of non-polar molecules:

1. Molecules with _____ atoms.
   The molecules of elements have identical atoms and therefore have pure covalent bonds. These bonds are non-polar and so the resulting molecules will also be non-polar. Examples of non-polar molecules include the gases, _____, _____,_____,_____,_____ and the solids _____ and _____.

However, molecules do not necessarily need to have non-polar bonds exclusively in order to be considered a non-polar molecule.

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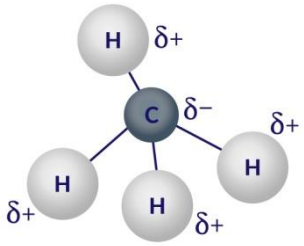
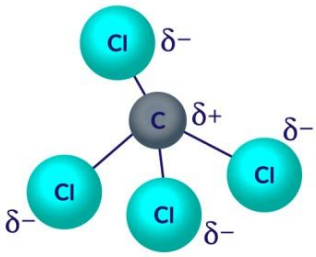
2. Molecules with different atoms (_____).

   Molecules made of different atoms will have polar bonds because the atoms will differ in their _____ (the ability to _____ bonding electrons). Molecules with polar bonds can be non-polar if the center of the negative charge _____ with the center of the positive charge.

   Methane shown to the right is a good example of a non-polar molecule, with polar bonds. The center of positive charge on each of the four _____ _____ coincides with the _____ _____ which is the center of negative charge. The center of positive (or negative) charge is defined as the point of _____ distance from each charge. It is right in the middle of the positive (or negative charges).



   The polar bonds in a molecule may be arranged in such a way that the overall molecule does not have a positive side and a negative side. If the polar bonds in a molecule are arranged _____ around the central atom, this causes the dipoles to _____ each other out. Tetrachloromethane pictured right is a good example of this.



The table below shows some common polar and non-polar molecules.

Substances that contain polar molecules	Substances that contain non-polar molecules
Hydrogen chloride HCl	Carbon dioxide CO_2
Phosphorous trichloride PCl_3	Oxygen O_2
Ammonia NH_3	Hydrogen H_2
Water H_2O	Nitrogen N_2
Dichloromethane CH_2Cl_2	Methane CH_4

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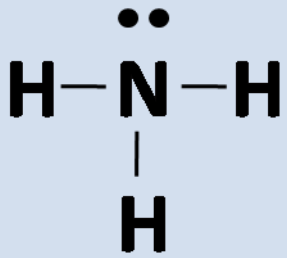
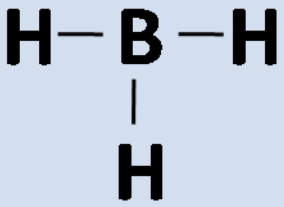
Practice problem:

The Lewis structures for two molecules are shown in the table below. Ammonia, NH_3 is polar, and borane BH_3 is non-polar. Justify this statement.

	Ammonia	**Borane**
Lewis Diagram		
Polarity	Polar	Non-polar

Justification:

VSEPR Theory and Predicting the Shape of Molecules

Valence shell electron pair repulsion (VSEPR) theory can be used to predict the shape of molecules. This theory uses the concept of _____ charges (in this case the _____ charged electrons) repelling each other. Electrons exist in _____, also known as electron sets, spread themselves out around an atom so that there is minimum _____ between them. This allows the molecules to be at their most _____. The areas which electrons occupy are also known as regions of electron density, electron clouds or electron domains.

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The position of the electrons determines how the atoms in a molecule _____ and gives the molecule its characteristic _____. This shape can be predicted from the _____ _____ and by counting the number of _____ _____ around the central atom.

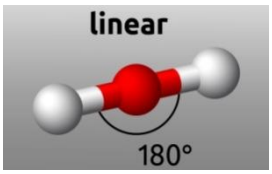
Establishing the number of electron sets

Electrons in a set cannot be separated without disrupting the bonds. An electron set can be made up of two _____ electrons of a lone pair, or the two _____ electrons of a single bond, or _____ bonding electrons in a double bond, or _____electrons in a triple bond.

Once the position of the electron sets has been established around the _____ atom, the other atoms are placed in the appropriate corners. The overall shape of the molecule is determined by the location of the atoms only, as the electron sets are not seen.

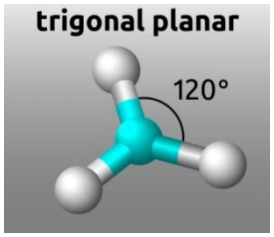
Two electron sets

When there are _____ electron sets, there will be a _____bond angle between the electron sets and the molecule will lie in a _____. This arrangement is called _____.

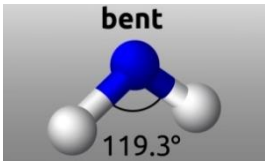


Three electron sets

When there are three electron sets, the electrons will repel each other so that they are pushed into the corners of an _____. The bond angle will be _____ with all three sets of electrons lying in the same plane. This arrangement is called _____.



In some cases, one of the three sets may be _____. These electrons must also be factored into the electron repulsion and so a similar bond angle is seen. This arrangement is called _____ and has a bond angle of _____.



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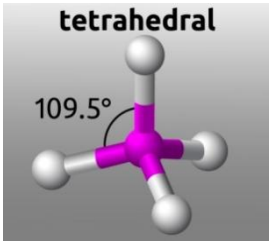
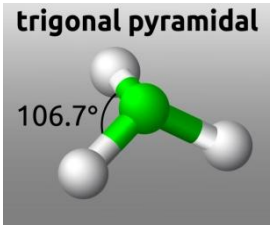
Four electron sets



When there are four sets of electrons then they repel each other so that they are directed into the corners of a _____. The bond angle will be _____and the electron sets will occupy _____ . This arrangement is called _____.



Just as is the case with three electron sets, sometimes one of the four electron sets is a _____. This arrangement is called _____ _____and has a bond angle of _____.

Determining Molecular Shape and Polarity

The following steps can be followed to determine the shape of a molecule and the resulting angles around the central atom.

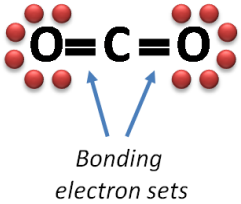
Step 1:
Draw the Lewis structure for the molecule.

Step 2:
Count the number of electron sets around the central atom to determine the arrangement of the electrons.

Step 3:
Count the number of bonding electron sets. Non-bonding electron pairs are not drawn in the final shape of the diagram.

Example 1: Carbon Dioxide (CO_2) Molecule

The electron dot structure of carbon dioxide is seen below:



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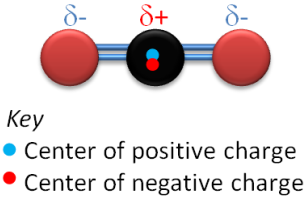
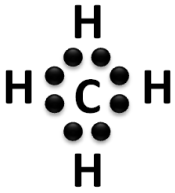
There are _____ electron sets around the central carbon atom. Each bonding electron set represents a double bond or 4 electrons. The two electron sets will repel each other until there is a much distance between them as possible, making the molecule _____ in shape and the bond angle _____. In carbon dioxide, the molecule the slightly negative (_____) oxygen atoms are evenly placed around the slightly positive (δ+)_____atom. The centers of negative charge and positive charge are both on carbon so the molecule is _____.

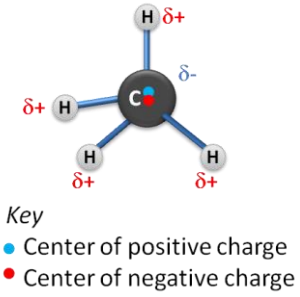


Example Two: Methane (CH_4) Molecule

The electron dot (Lewis) structure for methane is seen below:



There are_____electron sets around the central carbon atom with each electron set representing a single bond. Because the four electron sets repel each other, they must be as far away from each other as possible and are therefore pushed into the corners of a tetrahedron. So the four _____bonds will point to these corners and the molecule is called _____. In the methane molecule, the slightly positive (δ+)_____are evenly spaced around the negative (δ-)_____. This means that the center of positive charge and negative charge are in the same place - on the _____ atom and the CH_4 molecule has no overall _____ and is non-polar.



Example Three: Water (H_2O)

The electron dot (Lewis) structure for H_2O is:

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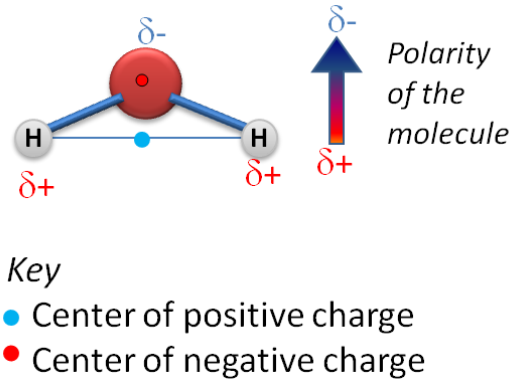
There are four electron sets around a central _____ atom. Two of these electron sets represent _____ bonds and the other two are _____ (non-bonding) pairs. These four electrons sets will repel each other so that they are as far apart as possible, directing each set into the corners of a tetrahedron as is seen in methane. However, unlike methane, two of these sets are lone pairs so instead of seeing the _____bonds of a tetrahedral, we only see _____ bonds from each of the hydrogen atoms (_____bonds) and the molecule is therefore _____.



The center of positive charge is _____ between the two hydrogen atoms, while the center of negative charge is on the _____atom. This means that water is a _____ molecule.

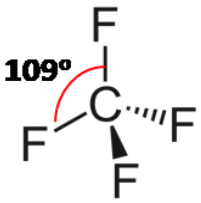
Conventions for drawing 3D wedge and dash structures

When drawing 3D molecules, the following conventions are used:

X— Y	both atoms in the plane of the page
X◄ Y	X in the plane of the page, Y is pointing 'out' of the page
X ıı··· Y	X in the plane of the page, Y is pointing 'into' the page

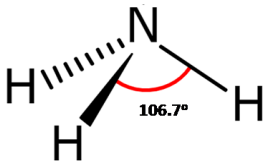
Example: The Shape of the CF_4 molecule

Carbon tetrafluoride (CF_4) has _____ sets of bonded electrons. Its Lewis diagram is shown to the right. Since the molecule is tetrahedral it will show _____ fluorine atoms in the plane of the page, one pointing _____of the page and one pointing _____the page.



Example: The shape of NH_3

Ammonia has _____ sets of electrons; _____ sets are bonding and _____ set is non-bonding. The shape of the molecule is _____with one N-H pair in the plane of the page, one pointing out of the page and one pointing into the page



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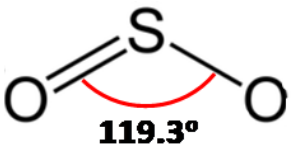
Example: The Shape of SO_2

Sulfur dioxide (SO_2) has _____ sets of bonded electrons and _____ pair of non-bonded electrons. Since sulfur dioxide is _____, the bonds will be _____ as the page, as seen in the diagram to the right.



Practice Problems:

1. Predict the shape, including the bond angle of Trichloramine (NCl_3). Use a wedge and dash diagram to support your answer.

   Answer:

2. Predict the shape and bond angle of boron trifluoride (BF_3). Draw the Lewis structure to support your answer.

   Answer:

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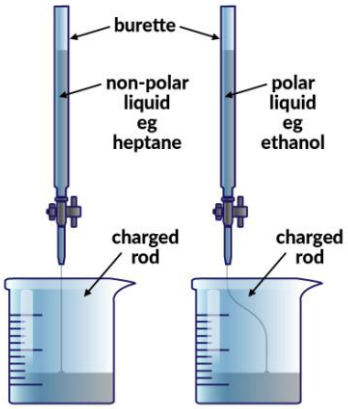
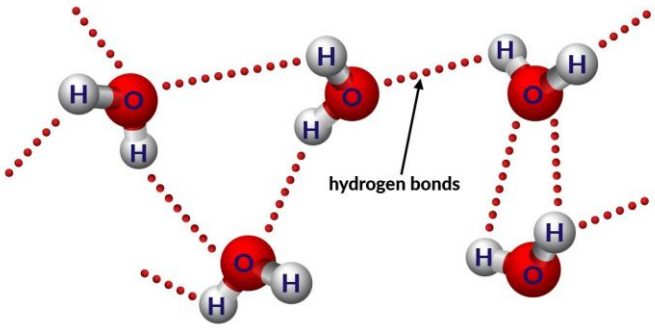
Testing for Polarity in Liquids

The molecules in liquids are _____. If they are placed near an electrically charged object, the _____molecules will align and be attracted to the charged object. This is because opposite charges are _____ one another. The stream of polar liquid (e.g. water) will be deflected _____ the charged object. This provides a test for polarity as _____liquids will continue to flow past the charged object _____ being deflected.



The Polarity of Water Molecules

Water molecules are _____, with polar _____bonds and a _____symmetry. Water has a higher melting and boiling point than is usual for a substance containing such low mass molecules. This is due to the fact that there is a relatively large difference in _____ between the hydrogen and oxygen atoms in water which produces strong attractive (_____) forces between the molecules called hydrogen bonds. These bonds require a considerable amount of _____ to break.



Because water is polar, it can also act as a solvent for some ionic compounds.

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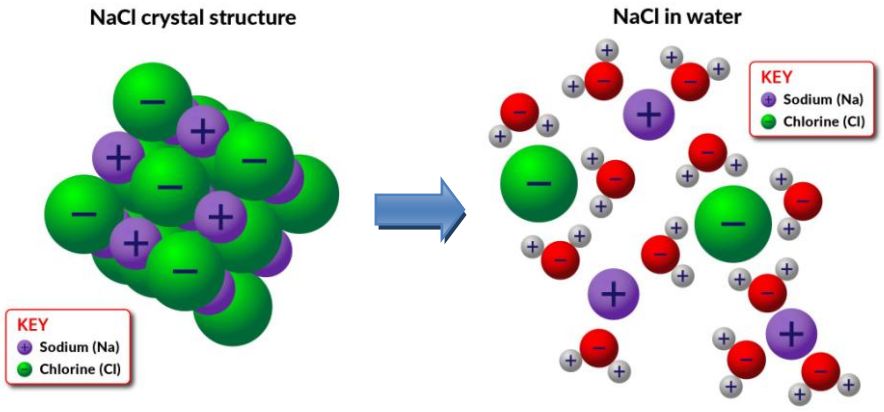
Dissolving

For an ionic solid to dissolve, the strong _____ bonds which hold the ions together must be broken. The ions are spread among the water molecules. The polar water molecules are attracted to the ions on the surface of the solid with the _____being attracted to the _____ end of the water molecule (i.e. the _____) and the _____ attracted to the _____ end (i.e. the _____). If the attraction between the ions and the water is _____ than the attraction between the cation and anion, then the solid will dissolve in water. The separated ions are surrounded by water molecules and form hydrated ions.



The energy required to break apart an ionic lattice (called the _____), differs for different ionic compounds. Ionic compounds are considered insoluble in water if _____ energy is required to separate the ions than can be gained by forming hydrated ions.

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Practice Problem:

Draw an annotated diagram to show how potassium iodide dissolves in water.